AEC Computing Facility

AEC RESEARCH AND DEVELOPMENT REPORT

PHYSICS NYO-7690

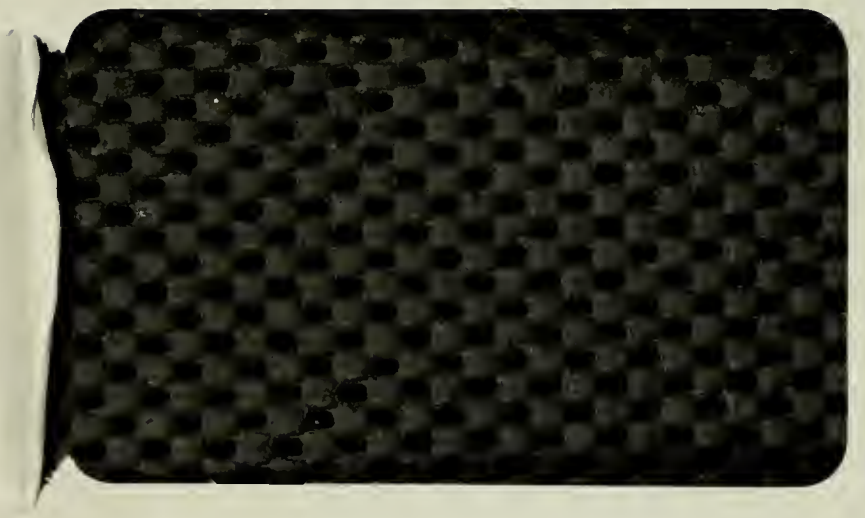
ANNUAL SUMMARY REPORT
OF
RESEARCH PROBLEMS INITIATED AT THE
INSTITUTE OF MATHEMATICAL SCIENCES
CONTRACT NO. AT(30-1)-1480

July 1, 1955 - June 30, 1956

institute of mathematical sciences

NEW YORK UNIVERSITY

NEW YORK, NEW YORK



AEC Computing Facility
Institute of Mathematical Sciences
New York University

PHYSICS NYO-7690

ANNUAL SUMMARY REPORT
OF
RESEARCH PROBLEMS INITIATED AT THE INSTITUTE OF MATHEMATICAL SCIENCES

CONTRACT NO. AT(30-1)-1480

July 1, 1955 - June 30, 1956

Issued
October 1, 1956

NYO-7690
PHYSICS

ABSTRACT

This report presents brief summary descriptions of research problems which were initiated and investigated at the AEC Computing Facility of the Institute of Mathematical Sciences at New York University during the period July 1, 1955 to June 30, 1956. Topics concern computing problems arising in applied mathematics or mathematical physics.

TABLE OF CONTENTS

Introduction. The Institute of Mathematical Sciences at New York University, of which the AEC Computing Facility is a part, has been authorized by the AEC to use some of the computing time set aside for research. The following sections provide brief descriptions of the problems which have been studied as part of this program during the past fiscal year. Since this is a summary report, the statements of the problems are not complete and do not contain much detail. In many cases the computational studies are parts of broader research programs.

Inquiries about any of the problems are welcomed.

Problem No. 1.12: The passage of a shock-wave over an obstruction in a channel

Investigators: Peter D. Lax and Glenn Lewis

When a shock wave travelling in a channel encounters a narrowing or an obstacle in the channel (see Figure 1), part of it is reflected, part transmitted. What is of interest is to calculate the strength of the transmitted and reflected waves, and the shape of the pressure pulse behind these waves.

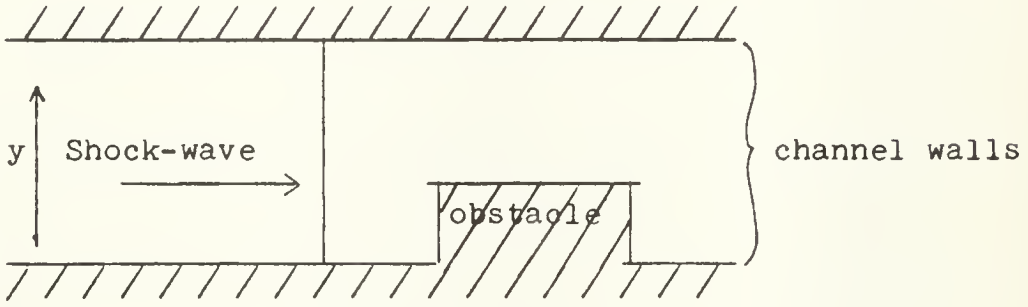


Figure 1.

The calculation of the effect of a blast wave on structures presents a similar problem. There the underlying domain is a halfspace as in Figure 2:

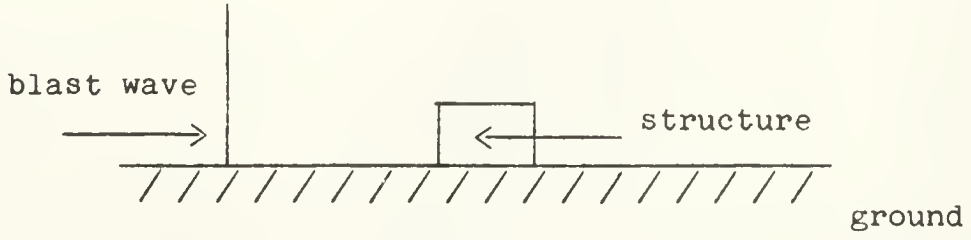


Figure 2.

The quantity of interest here is the distribution of pressure over the structure as a function of time.

The method of calculation: Eulerian coordinates were used, and the equation of state was taken to be a γ-law, $\gamma = 1.4$. The equations of motion were written in conservation form:

$$\rho_t + m_x + n_y = 0$$
$$m_t + (um+p)_x + (vm)_y = 0$$
$$n_t + (un)_x + (vn+p)_y = 0$$
$$E_t + (u(E+p))_x + (v(E+p))_y = 0.$$

Here m and n abbreviate momenta in the x and y direction, and E is total energy per unit volume

$$m = \rho u,\ n = \rho v,\ E = \rho e + \frac{1}{2}\rho u^2,\ e = \frac{p}{\rho(\gamma-1)}\ .$$

ρ, m, n and E were the unknown functions used in the computations; the others were expressed as functions of them. A rectangular grid staggered in time was used, i.e. at even time cycles all quantities were expressed at even lattice points, at odd times at half points (see Figure 3).

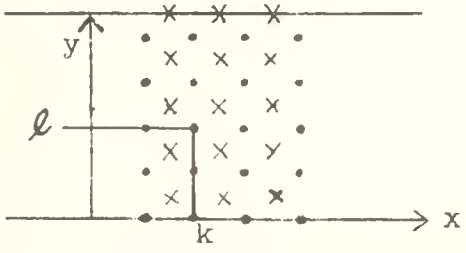


Figure 3.

• position of quantities at even time step

× position of quantities at odd time step

Time derivatives were replaced by averaged forward difference quotients, i.e. for n odd:

$$\Delta_t \rho \sim \rho^{n+1}_{k,\ell} - \frac{\rho^n_{k-1/2,\ell-1/2} + \rho^n_{k+1/2,\ell-1/2} + \rho^n_{k-1/2,\ell+1/2} + \rho^n_{k+1/2,\ell+1/2}}{4}$$

and similarly for n even. Space derivatives were replaced by centered difference quotients:

$$\rho_x \sim \frac{\rho^n_{k+1/2,\ell+1/2} - \rho^n_{k-1/2,\ell+1/2}}{2\Delta x} + \frac{\rho^n_{k+1/2,\ell-1/2} - \rho^n_{k-1/2,\ell-1/2}}{2\Delta x}$$

At boundary points reflected values were used at the lattice points which fell outside the flow region, i.e., the value of ρ, E and p was reflected while the value of u, v was changed so as to preserve the tangential flow velocity and reverse the normal velocity.

Initial configuration: Two regions with constant states connected through a straight shock, as shown in Figure 1. The pressure ratio was 3:1.

Stability criterion: A useful criterion of Friedrichs for stability was employed, which for the scheme under consideration requires that

$$\lambda|u| + \mu|v| + c\sqrt{\lambda^2+\mu^2} \leq 1,$$

where c is sound speed, and λ and μ abbreviate

$$\lambda = \frac{2\Delta t}{\Delta x} \quad , \quad \mu = \frac{2\Delta t}{\Delta y} \quad .$$

As the mesh was traversed during the calculation, the current value of Δt was checked at each point and enlarged if necessary for the next time cycle. This comparison was arranged so as to avoid the extraction of square roots.

Organization of data in the machine: The values of the hydrodynamical variables along the lattice points on one vertical line (i.e. x = const.) were stored in one block on tape 1. At any given time there were data from two neighboring vertical lines (the left and the right) in the internal memory, from which the new values at the line in between were computed. These new values were dumped on tape 2; then the contents of the right line were transferred to the left line internally; and then the right line was filled from the next block on tape 1. In the next time cycle the mesh was swept from right to left, reading from tape 2 and writing on tape 1.

All calculations were carried out in fixed decimal.

Output: Pressure, density, flow speed and flow angle were tabulated separately to three significant figures, in floating decimal notation. The tables were replicas of the channel; each entry appeared over the lattice point whose value it represented.

Results: 50 time cycles were ground out, in about 2 1/2 hours. The shock, which initially started at some distance from the obstacle, was just over the edge. There was an increase in pressure against the obstacle as the reflected shock was beginning to build up. The isobars plotted around the diffracting corner presented the kind of pattern one would expect on the basis of acoustic theory.

The calculation so far has given no inkling of the strength of the reflected and transmitted shocks. We are optimistic through that if run long enough the method will furnish this information.

Problem No. 1.13: Underwater explosion bubble oscillations (Bubble)

Investigators: L. K. Brathwaite, P. Fox, J. B. Keller

When an explosive detonates underwater it is immediately changed into a gas at high pressure. This gas, called the bubble, expands until its pressure equals that of the surrounding water, but inertia causes it to overexpand. Finally it comes to rest momentarily at a lower pressure but then the surrounding liquid recompresses it. Then it expands again and this process repeats a number of times before the bubble finally breaks up or vents at the surface.

The usual theory of these oscillations treats the bubble as a sphere and assumes the water to be incompressible. This theory has been modified by Dr. J. B. Keller and Dr. I. I. Kolodner to take account of the compressibility of the water. It then yields damped oscillations of diminishing period, in agreement with experimental observations. This modified theory is described in "Underwater Explosion Bubbles I. The Effect of the Compressibility of the Water" IMM-NYU No. 191.

The theory leads to a non-linear second order ordinary differential equation for the bubble radius as a function of time. This equation was programmed and coded for solution on Univac by Dr. P. Fox, M. Billings and L. Brathwaite. A number of radius-time curves were computed. These curves, together with the theory, will be published in the Journal of Applied Physics in an article by J. B. Keller and I. I. Kolodner entitled "Damping of Underwater Explosion Bubble Oscillations."

Problem No. 1.16: Solution of elliptic difference equations (Pogo)

Investigators: R. Dykaar, K. Gordis, H. B. Keller

A large class of finite-difference approximations to linear elliptic partial differential equations (i.e. Laplace's equation, equations of neutron diffusion, elastic plate and membrane equations, etc.) can be written as a system of linear algebraic equations in the form

$$(1) \qquad (I - H)\,\underline{\Phi} = C \quad .$$

Here I is the unit matrix; H is a square matrix whose elements depend upon the mesh spacing, the coefficients of the original equation, and the method of differencing employed; C is a column vector whose components depend upon the mesh spacing, inhomogeneous terms in the original equation and the boundary conditions; and $\underline{\Phi}$ is a column vector whose components are the unknown numerical approximation to the solution.

The order of this system is essentially the number of mesh points in the domain under consideration. Thus for problems in two or more dimensions the system (1) may be of such large order that general matrix methods of solution are impractical or perhaps unacceptably inaccurate. However, the origin of these equations leads us to expect that H may have a special form with many zero elements, and accordingly some particular methods for the solution of (1) have been presented.[1] The Pogo program is an attempt

1. S. P. Frankel: M.T.A.C. 4, 65 (1950).

to investigate and improve methods for the numerical solution of these special forms of the system (1).

In particular the class of methods under consideration are iterative techniques and may be generally described as follows: The coefficient matrix is "split" into the difference of two matrices

$$I - H = A(\alpha) - B(\alpha) , \tag{2}$$

whose elements are functions of some real parameter, α, in such a way that $|A(\alpha)| \neq 0$. Then from some initial guess at the solution vector, $\underline{\Phi}_0$, we define a sequence of approximations, $\underline{\Phi}_n$, by

$$A(\alpha)\, \underline{\Phi}_n = B(\alpha)\, \underline{\Phi}_{n-1} + C . \tag{3}$$

If this sequence converges, the limit vector is clearly the solution of (1). We seek "splittings" of the form (2) and corresponding values of the parameter, α, for which convergence of the sequence (3) is assured and is as rapid as possible. An important restriction to be imposed is that the resulting equations (3) may be solved in some "simple" straightforward manner.

Many of the standard iterative procedures for solving such systems are easily cast into the above form and their theoretical analysis becomes simple and elegant. These methods also suggest quite naturally other splits which are under investigation. The neighbor relationships in the difference equations and methods of sweeping the mesh dictated by efficient use of digital computers suggest still

more splits which are to be examined.

For any split of form (2) the theoretical investigation of convergence requires a determination of the eigenvalue of largest absolute value of the matrix $A^{-1}(\alpha)B(\alpha)$. To compare rates of convergence of two different schemes we need only a comparison of these eigenvalues. However, for some splittings which have been proposed and used successfully the eigenvalues are unknown or have a complicated dependence on various quantities (i.e. mesh spacing, α, number of mesh points, etc.). Such schemes are being studied by means of numerical experiments in which convergence rates are observed and the maximum eigenvalues and best values for α are computed approximately. As a basis for comparison these same experiments will be conducted for a scheme (probably extrapolated Liebmann) whose theoretical properties are well known.

At present the Pogo program is considering second order equations in two dimensions with second order difference approximations on full rectangular meshes. Some recent investigations by H. J. Greenberg indicate rather clearly that much improvement in efficiency may be obtained by considering staggered meshes. The possibilities offered by higher order difference approximations also seem promising. It is hoped that some of these considerations will be included in future investigations.

Problem No. 1.18: The treatment of contact discontinuties in a Eulerian calculation (Interface)

Investigators: R. Buchal and P. D. Lax

Contact discontinuities in compressible flows behave like discontinuities of solutions of linear equations. The similarity is present in finite difference calculation and has this effect: the width of the transition region spreads like the square root of the number of time cycles, unless special cognizance is taken of the presence of the contact discontinuity. If the contact discontinuity separates two fluids of verydifferent densities, this diffusion across the interface causes a very large distortion. In Lagrange coordinates it is possible to prevent the diffusion of the discontinuity by an appropriate differencing of the equations; this is not possible in Euler coordinates. The reason for it is that in Lagrange description the position of the contact discontinuity is unchanged in the grid; in Euler coordinates it is not.

In our sample calculations we tried out some specific measures to prevent diffusion. Two steps are involved:

a) keeping track of the contact discontinuity;

b) devising special difference schemes to be used at points whose neighbors straddle the discontinuity line.

These extra operations consume negligible time compared to the main body of the calculation.

So far the method has been tried on some one-dimensional problems involving the impinging of a shock of constant strength on an interface. The method furnished the transmitted and reflected shocks fairly accurately.

We contemplate trying the method for a two-dimensional flow involving shear.

Problem No. 1.19: On the rates of convergence and the stability properties of finite difference solutions to hyperbolic systems. (Difference)

Investigator: W. Gersch

The objective of this work was to investigate the characteristics and relative merits of the "centered" and the "staggered" finite difference schemes as they are applied to first order hyperbolic systems. Particular attention was focused on the rates of convergence and the stability properties of both schemes.

The scheme referred to as a centered scheme is one in which the time and space derivatives are centered, the staggered scheme has derivatives centered in space and staggered in time. Both schemes are applied to rectangular nets.

These schemes were applied systematically to the study of a one dimensional time dependent compressible fluid flow problem. Machine calculations were made in an attempt to provide experimental results to supplement an analytic examination of the finite difference schemes.

A theoretical analysis of the application of each of the finite difference schemes to the hyperbolic system yields criteria for the determination of the mesh ratio to insure convergence and stability of the numerical computations. In addition it is possible to extract a measure of the error of approximation of the finite difference scheme to the partial differential equation.

The motivation for examining these schemes is straightforward. The convergence and stability of the staggered

scheme have been analyzed quite generally. The finite difference approximations to the partial differential equation for the staggered scheme are correct to order of the square of the mesh width $O(\Delta^2)$. The centered scheme which lacks a rigorous general convergence proof is correct to within $O(\Delta^3)$, and therefore suggests closer approximation to the solution of the partial differential equations. It was thought desirable to get some experimental evidence on the merits of each scheme.

The case examined experimentally was an initial value problem where the first derivatives do not satisfy a Lipschitz condition. (This case has as yet not been analyzed successfully). An investigation of the convergence and stability characteristics of finite difference schemes was made and attention was focused on the growth and decay of errors both within a disturbance region and in a region of quiet.

The experimental results suggest that the centered difference scheme does in fact give a generally closer approximation to the solution of the partial differential equation than the staggered scheme. As expected, the errors do propagate along the characteristics. Each scheme exhibits a particular behavior at the characteristic crossings and the machine calculations were valuable here in enforcing a speculation concerning the random insertion of errors.

An additional important observation was that it appears that there is an optimum practical closeness to the numerical solution of nonlinear hyperbolic equations whose derivatives do not satisfy a Lipschitz condition and that it is not desirable to attempt an exchange of an increase of computing time for a closer numerical approximation.

One disquieting result is that neither scheme exhibited monotonic convergence characteristics within the disturbance region. This suggests that additional computing be done for better behaved cases to provide reassurance that the first impression, that the centered scheme is in fact superior to the staggered scheme for nonlinear hyperbolic systems, is on a firmer footing.

Problem No. 1.20: Numerical methods tests

Investigator: R. D. Richtmyer

Under this heading is grouped a number of investigations which have been going on at various times during the past two years, in part under other numbers (NYU 1.15 and LASL 6.3). Most of the results have been presented at various seminars and meetings. A few of them will be described in a forthcoming book on Numerical Methods for Initial-Value Problems.

1.20.1 Pseudo-viscosity method for shocks. When finite-difference methods are applied to fluid-dynamics calculations using the pseudo-viscosity method (Von Neumann and Richtmyer, Journal of Applied Physics, 1950) the questions of accuracy and stability become important and cannot be completely settled by analytical methods. A code was prepared for following a one-dimensional running wave (shock) in Lagrangean coordinates for various values of a) shock strength, b) time increment, c) ratio of specific heats, d) coefficient of pseudo-viscosity. The machine gives profiles of pressure, volume, entropy, fluid velocity and obtains the shock speed and asymptotic values of pressure and the like by least-squares and averaging.

It was found that for reasonable values of the above parameters the shock speed agrees with the Rankine-Hugoniot value to a fraction of a percent; the pressure rise occurs in two to three space intervals; and behind the shock the pressure oscillates about the correct value with oscilla-

tion amplitudes of 1 to 5 percent (depending on conditions) of the pressure jump. The results indicate that the method should be satisfactory for many problems.

Stability was investigated recently, using this code to determine the critical value of the time increment for various shock strengths. The results agree qualitatively with the approximate theoretical stability criterion of Von Neumann and Richtmyer, but the equations are slightly less stable for weak shocks and slightly more stable for strong shocks, than was expected.

1.20.2 "Imp". A family of implicit finite-difference equations was applied to the solution of the non-linear parabolic equation

$$\frac{\partial}{\partial t} u = \frac{\partial^2}{\partial x^2} u^{\alpha}$$

where α is a positive integer (= 5 for the cases run so far). Initial and boundary values are taken from a certain analytic solution. The machine prints the approximate and exact solutions in parallel columns every ten cycles. (The exact solution is obtained by Newton-Raphson inversion of a power series). The agreement is very good, considering the coarseness of the mesh used, and the stability requirement agrees well with the one obtained by the usual heuristic arguments.

1.20.3 Diophantus. If ξ is an irrational number, the sequence x_n = fractional part of $n\xi$ is asymptotically uniformly distributed in the internal $0 < x < 1$. There is

reason to believe that for certain choices of ξ the fluctuations of this distribution are smaller than would be the case for a random sequence. Because of possible application to model sampling("pseudo Monte Carlo"), the mean-square fluctuations were computed for sequences x_n, with n running up to several thousand, for various choices of ξ. Double precision arithmetic was used. The fluctuations are noticeably small when ξ is a quadratic or cubic irrational or a rational linear function of e.

1.20.4 n^{th} root. A double-precision root extractor for use with "diophantus".

1.20.5 Monte Carlo pilot run. Early, preliminary version of the resonance escape calculation.

1.20.6 2-dimensional shock. (originally LASL 6.3)

A heartbreakingly unsuccessful attempt to develop a partly Eulerian, partly Lagrangean method of treating fluid-dynamical problems in two space variables and time.

1.20.7 Hex relaxation convergence test. The over-relaxation or "extrapolated Liebman" method was applied to elliptic problems of the Helmholtz type in two space variables using a hexagonal net of points. Automatic rescaling as the residual is quenched allows determination of the fundamental mode and optimum over-relaxation factor with any desired accuracy. Intended mainly for use with 1.20.8 below.

1.20.8 2-dimensional diffusion. Various implicit schemes of allegedly high accuracy, using a hexagonal space net, were applied to the diffusion equation in an attempt to find improved methods for solving the multi-dimensional age-diffusion equation in reactors. Three difference schemes, using 21 points, 14 points, and 9 points, respectively, were investigated for a problem in which the exact solution is known and could be computed by the machine (by power series) for comparison. The improvement by use of "high-accuracy" formulas was disappointingly small.

1.20.9 Stability demonstration. Mainly for instruction purposes. A simple heat flow problem is solved by the explicit equation. The time increment can be chosen above or below the stability limit. The machine also calculates the exact solution by Fourier series.

1.20.10 Neutron transport integral equation. The odd solutions of the eigenvalue problem

$$\lambda\Phi(s) = \int_{-a}^{a} E(\beta|s-r|)\Phi(r)dr$$

where

$$E(x) = \int_{|x|}^{\infty} (e^{-y}) \frac{dy}{y}$$

are related to the normal modes of neutron multiplication (or decay) in a one-group bare-sphere problem with isotropic scattering. An iterative scheme was coded whereby: a) the first two odd eigenfunctions (corresponding to the two

highest values of λ) are found concurrently, b) β is automatically adjusted during the calculation to make the highest eigenvalue converge to unity, c) in calculating the fundamental eigenfunction, Tchebyscheff polynomials are used to suppress the higher eigenfunctions. The integral is evaluated as a Stieltjes integral to avoid inaccuracy because of the logarithmic singularity of the integrand. Even when a quite fine mesh is used, the method converges rapidly. The principal use is to provide accurate standards of comparison for the asymptotic behavior of the solutions of the transport equation given by 1.20.11 below.

1.20.11 Method of characteristics for the time-dependent transport equation. (Continuation of work started at Los Alamos). The transport equation for a bare sphere of isotropically scattering material is

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{\partial}{\partial x} + \sigma\right)\psi(x,y,t) = \sigma\varphi\left(\sqrt{x^2+y^2},t\right) ,$$

where

$$\varphi(r,t) = \frac{1}{2r}\int_{-r}^{r} \psi\left(x,\sqrt{r^2-x^2},t\right) ,$$

and is to be solved in the semicircular region $y \geq 0$, $x^2+y^2 \leq a^2$ with the boundary conditions

$$\psi\left(-\sqrt{a^2-y^2}, y, t\right) = 0 \qquad (0 \leq y \leq a) .$$

A direct integration method which follows the characteristics (these are the lines y = constant, $x-ct$ = constant) has

been coded for test of the method. Non-trivial analytic solutions for comparison are not known, but information can be obtained by successive refinement of the mesh and by comparison of the asymptotic form of the solution with functions obtained from 1.20.10. Results so far indicate that the method is accurate enough and fast enough that it may compte with other methods, such as the S_n method of Carlson, for some purposes.

Problem No. 1.22: Schrodinger wave equation (Schemer)

Investigator: M. Salkoff

The purpose of this project is to set up a program for solving Schrodinger's radial equation for potentials that are repulsive near the origin. The solutions for such a potential are of interest in scattering problems. The problem under study here is that of low energy inelastic collisions between H_2 molecules. This problem has been examined by E. Bauer in research report CX-17, published by the Institute of Mathematical Sciences. In that report, the WKB approximation is used to solve the radial equation. It is felt that the more accurate solutions obtained by the Univac will determine the usefulness of the approximation employed in CX-17.

The radial equation can be put in the form

$$(1) \qquad \frac{d^2f(r)}{dr^2} + [k^2 - \frac{2mv(r)}{h^2} - \frac{\ell(\ell+1)}{r^2}]f(r) = 0.$$

Solutions are needed for various values of k^2, which is proportial to the energy of the incident H_2 molecule, and ℓ, which is proportional to its angular momentum. The solutions obtained are used to calculate the inelastic cross-section by means of simple perturbation theory and some appropriate perturbation potential. This cross-section will then be compared with that obtained by Bauer in CX-17 using the WKB approximation. The quantity of

interest is the matrix element of the perturbation potential between the initial and final states of the system. The latter are in effect the solutions of equation (1) for the initial and final energies of the incident particle. Since many values of ℓ are needed in order to calculate the cross-section at the energies considered, the Univac is needed for the laborious series of integrations.

A Runge-Kutta integration scheme was used to solve equation (1). The solutions so obtained were checked both by hand computations and by comparing with the WKB method which is fairly accurate for relatively large r. Both methods of checking agreed closely with the Univac results. As a further check, two intervals of integration were used to solve equation (1), for one set of values of k^2 and ℓ. Comparison indicated that the solutions are good to at least four significant figures when the solution is of order unity.

The Univac program in its present state does not yet give the correct value of the perturbation matrix element although the solutions of equation (1) do seem to be correct, as indicated above. The final total cross-section calculated by means of these matrix elements does not vary correctly with energy. (The variation of cross-section with energy is well known, but the quantitative details are not.) The error has not yet been found.

Problem No. 1.23: Complex eigenvalued differential equation (Friedman)

Investigators: S. Schechter

This is concerned with the problem of finding a numerical solution to the following analytic problem:

Find $\min_{w} \operatorname{Im} \{ \lambda(w) \}$ where $w(t,\lambda)$ is a solution of

$$(*) \quad \begin{cases} \dfrac{d^2w}{dt^2} + \left(k^2(t) - \dfrac{\lambda}{t^2}\right) w = 0 & (1) \\ \lim_{t \to \infty} \left| \dfrac{dw}{dt} - iwk_o \right| = 0 & (2) \\ w(a,\lambda) = 0 & (3) \end{cases}$$

where $k^2(t) = k_0^2 \left(1+\alpha e^{-\beta(t-a)}\right)$, and a, k_o, α, β are given positive constants.

This problem arose out of investigations in the theory of tropospheric refraction of radio waves.

It can be shown that there exists a unique solution to the above problem without condition (3). We may therefore regard the λ_i as eigenvalues with the property: $w(a,\lambda_i) = 0$. Since $w(t,\lambda)$ is analytic in t and λ for $t \geq a > 0$, these λ_i are isolated.

It can also be shown that if a solution of (*), (w,λ) exists, then

$$\operatorname{Im} \{ \lambda \} \geq \frac{2|\lambda|}{A(e^{2|\lambda|/k_o a} - 1)}$$

where $A = e^{2\alpha k_o/\beta}$.

One method that has been used in eigenvalue problems arising from two-point boundary conditions is to write the equation in difference form and solve a matrix problem. As an experiment to check this method the problem $w'' + \lambda^2 w = 0 \quad w(o) = w(a) = 0$ was solved by Givens' code for various mesh spacings. The results showed that the eigenvalues with the smallest magnitude yielded about 3 digits accuracy for 37 mesh points but those with largest magnitude had over 100 percent error. Nevertheless one can use several of these values as initial guesses for some integration schemes.

An integration scheme is now being coded which will integrate (1) from two different starting points. One point is in a neighborhood of infinity and the initial values are obtained from an asymptotic expression for w. With a choice for λ one would seek a point $t = a$ such that $w(a,\lambda) = 0$. The other point of departure is to start at $t = a$ with condition (3) and $w'(a,\lambda) = c$ prescribed. The outward integration would check for condition (2) in the neighborhood of $t = \infty$.

Problem No. 1.24: Solution of integral equation (Toff)

Investigators: G. E. Forsythe, M. Salkoff

In order to solve the integral equation

$$f(x) = g(x) + \int K(x,x')\, f(x')dx' \tag{1}$$

inversion of the integral operator by matrix methods suggests itself. This may be a very time-consuming procedure, however. Various gradient methods of solution of operator equations of the form

$$V(x) = Lu(x) \tag{2}$$

have been investigated.[1] The present project was undertaken in the hope that such a method might yield a solution of equation (1) more rapidly than matrix inversion. The basis of such a hope lies in the fact that gradient methods of solution of operator equations do not explicitly solve for the inverse of the operator. Rather, the solution vector itself is found by an iterative process, and this may entail fewer multiplications and consequently less time than matrix inversion.

The following iteration scheme was originally used: Suppose

$$V = L\,u \;;\; V \text{ given, } u \text{ sought} \tag{3}$$

Take

$$V_o = V \tag{4}$$

---

1. Forsythe and Forsythe, NBS report AMS 39, Sept. 1954, p. 55, and bibliography therein.

(5) $V_n = V_{n-1} - L\,u_n$ where

(6) $u_n = \lambda_n\, L^T\, V_{n-1}$ (L^T = L transpose).

To determine λ_n, take

(7) $(V_n, L\,u_n) = 0$ where the brackets represent an inner product.

Using (5) for V_n and (6) for u_n, we have

$$(V_{n-1} - \lambda_n\, L\, L^T\, V_{n-1},\ L\, L^T\, V_{n-1}) = 0$$

or

$$\lambda_n = \frac{(L^T V_{n-1}, L^T V_{n-1})}{(L\, L^T V_{n-1}, L\, L^T V_{n-1})} = \frac{|L^T V_{n-1}|^2}{|L\, L^T V_{n-1}|^2} \quad .$$

It follows that

$$\sum_{i=1}^{n} u_i = L^{-1}(V_o - V_n)$$

and

$$\lim_{n\to\infty} \sum_{i=1}^{n} u_i = L^{-1} V_o = L^{-1} V = u$$

provided

$$\lim_{n\to\infty} L^{-1}\, V_n = 0 \ .$$

Two slight modifications were introduced in the hope of speeding up the convergence of the iteration procedure: (1) δ^2 - acceleration of the remainder vectors V_n; and (2) introduction of an arbitrary multiplicative factor β in the expression for λ_n, which is varied from 1 to

about 0.8.

The results were not very good, and the method as it stands does not compare favorably with matrix inversion. Nevertheless, results obtained under modification (2) above are similar to those obtained by S. Stein,[2] even to the best value of β.

---

2. Ibid., especially references (7) and (11) therein.

Problem No. 1.25: Numerical methods for general transport equations (Tramp)

Investigators: H. B. Keller, B. Wendroff (of L.A.S.L.)

Many problems concerned with weapons, weapons effects, shielding and related fields require the solution for the density ϕ, of some type of particles as defined by the transport equation in the general form

$$(1)\quad \left\{ \frac{1}{v}\frac{\partial}{\partial t} + \underset{\sim}{\omega}\cdot\underset{\sim}{\nabla} + \sigma(t,\underset{\sim}{r},v) \right\} \phi(r,\underset{\sim}{r},v,\underset{\sim}{\omega}) = F(\phi,t,\underset{\sim}{r},v,\underset{\sim}{\omega}).$$

Here $\underset{\sim}{r}$ is a position vector, v is the speed of the particles, $\underset{\sim}{\omega}$ a unit vector in the direction of motion of the particles, σ is a cross-section for the loss of particles, say by fission, scattering, emission or any combination of these processes. Since analytic solutions of such an equation are known only for extremely specialized cases, efficient numerical methods for the solution of these equations are of great value. The present program is an attempt to investigate, devise and improve methods for treating such problems.

As equation (1) contains seven independent variables numerical procedures to be used on existing or proposed computers must be specialized to less general configurations or physically simpler phenomena (i.e. steady states, few velocities, weak angular dependence, etc.) In particular, we consider cases of spherical symmetry or infinite plane symmetry in which case the independent variables are

reduced to four: t, r, v, μ, where r is radius or distance from the plane of origin and μ is the cosine of the angle between position vector and particle velocity. A steady state form of the resulting equations (i.e. ϕ independent of t) has been studied theoretically and numerically in some detail (in the case of plane geometry where F represents only scattering and/or emission). This program, called Achilles, was successful in that a stable convergent numerical procedure was obtained[1] and used in experimental and practical problems. In the present work we consider spherically symmetric one-velocity problems (i.e. v enters only as a fixed parameter) with scattering or emission. The extension of methods devised in this study to plane geometries is immediate.

A basic approach to the resulting equation, in this case

$$(2)\quad \left\{ \frac{1}{v}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial}{\partial \mu} + \sigma \right\} \phi(t,r,\mu) = F(\phi;r,\mu) ,$$

has been presented by Bengt Carlson[2]. We have modified his formulation and are studying the stability and con-

---

1. H. B. Keller and J. Heller: On the numerical integration of the neutron transport equation, AEC Computing Facility, Institute of Mathematical Sciences, New York University, NYO-6481.

2. B. Carlson: Solution of the transport equation by S_n approximations, Los Alamos Scientific Laboratory, LA-1891.

vergence of the resulting scheme. Numerical experiments are also being conducted to determine the best practical procedures and to examine various features which do not, at present, seem amenable to theoretical analysis.

Our approach has been to difference equation (2) in the μ-variable first. The resulting differential-difference equations are then seen to form a hyperbolic system of first order linear partial differential equations, the number of dependent variables being equal to the number of μ-points taken in the interval $-1 \leq \mu \leq 1$. These equations are then differenced, essentially as in (2) but with some important simplifications, such that no restrictions are placed on the mesh ratio, $\Delta r/\Delta t$. It is shown in the plane case and in the spherical case excluding the origin that the difference scheme for the hyperbolic system is stable and convergent. Attempts at extending the method and analysis to include the origin are in progress. Numerical experiments show no instabilities at the origin but, possibly, some other peculiar behavior. The question of convergence of solutions of the difference-differential equations to those of the transport equation (2) is more difficult and will be examined both theoretically and numerically.

An important consequence of these investigations has been the development of an unconditionally stable

explicit difference scheme for hyperbolic systems of first order quasi-linear partial differential equations. These results will be described in detail in the near future.

Problem No. 1.26: Meteorological mixed boundary-initial value problem (Meteor)

Investigators: P. Fife, E. Isaacson, J. J. Stoker

In a general program for developing numerical methods for solving hyperbolic partial differential equations in two or more dimensions, one of the first difficulties that must be overcome is the proper treatment of boundary data in the mixed boundary-initial value problem. We have begun an investigation of how to treat the boundary conditions in a meteorological problem that was formulated by J. J. Stoker.

The problem is to determine whether it is possible to predict the behavior of a wedge of cold air on the earth's surface by solving numerically an initial-boundary value problem involving three equations derived by Stoker as an approximate description of the situation. The three equations are

$$u_t + uu_x + vu_y + Ah_x = \lambda v$$

$$v_t + uv_x + vv_y + Ah_y = \lambda\left(\frac{\rho'}{\rho} u' - u\right)$$

$$h_t + (uh)_x + (vh)_y = 0,$$

where u and v are the east and north components of the (cold) wind velocity; h is the height above the ground of the discontinuity surface between cold (below) and warm (above) air; x and y are distances with respect to an orthogonal coordinate system on a plane

tangent to the earth's surface, the x-axis running east, the y-axis running north; ρ and ρ' are densities of the cold and warm air; u' the warm air velocity; and

$$A = g(1 - \frac{\rho'}{\rho}) \quad ,$$

$$\lambda = 2\,\omega \sin \varphi \quad ,$$

where ω is the angular velocity of the earth and φ is the latitude. The problem is somewhat novel since the domain in which the solution is sought is bounded on the south by a "free boundary".

The procedure has been to put these equations in a difference form and carry out the calculations for a specific region of the earth's surface, bounded on the east, west, and north by fixed boundaries and on the south by the moving cold front. Various runs are being made corresponding to several hours each in actual time, to determine the effect of (1) the method used of handling the free boundary; (2) the number and type of boundary conditions applied to the fixed boundaries, and (3) the initial data used.

So far runs have been carried out using two distinct methods of treating the free boundary, the results showing little difference. A prescription of fixed u, v, and h on the east and west boundaries has been used always, but as for the north boundary, runs have been made with

(vh) prescribed there as a function of x alone, as well as runs prescribing u, v, and h as fixed. These both have produced somewhat unsatisfactory results. A run is shortly to be made in which $v = 0$ is the only "artificial" boundary condition to be prescribed on the north (the other conditions being derived from the equations).

In the initial conditions used, the deviation from an equilibrium pattern (a perfect wedge with $u \equiv$ const., $v \equiv 0$) has been localized in the middle of the region. This deviation has usually been a ridge or a trough in the wedge of cold air.

Problem No. 1.27: Singular integral equation (Ship)

Investigators: K. Grossman, E. Isaacson, A. Peters, J. J. Stoker

We have begun a program to develop methods that will be appropriate for the numerical solution of singular integral equations of the first kind.[1]

For example, we want to find the solution $\varphi(x,y)$ defined in the domain D with boundary B, such that

$$(1) \quad K(x,y) = \iint\!\!\!\!\!\!\diagup_{D} \frac{(\xi-x)\varphi_{\xi}(\xi,\eta)+(\eta-y)\varphi_{\eta}(\xi,\eta)}{[(\xi-x)^2+(\eta-y)^2]^{3/2}} d\xi d\eta$$

where $K(x,y)$ is given and the integral is evaluated as a Cauchy principal value integral. That is,

$$\iint\!\!\!\!\!\!\diagup_{D} = \lim_{\epsilon \to 0} \iint_{D_\epsilon} \text{, where}$$

D_ϵ is the subset of D which is obtained by deleting a circle of radius ϵ centered at the singular point (x,y).

Owing to the fact that equations such as (1) do not have unique solutions, we are able to impose another restriction on $\varphi(x,y)$. J. J. Stoker and A. Peters propose the boundary condition $\varphi(B) = 0$ for their physical problem.

Prior to starting on the two-dimensional problem, we are studying a one-dimensional integral equation, for which we are developing methods that will be useful in

---

1. These equations arise in the study of the motion of thin floating ships in the work of J. J. Stoker and A. Peters. They have suggested the problems we are considering.

problems of higher dimension.

The equation

(2) $K(x) = -\frac{1}{\pi} \oint_{-1}^{+1} \frac{\varphi(t)}{t-x}\, dt$ with the auxiliary

relation, to ensure uniqueness,

(2a) $\int_{-1}^{1} \varphi(t)\, dt = 0$, has been solved numerically.

Method A: We tried the simplest finite difference approximation for the integral in (2) based on the representation which exhibits the boundary behavior, $\varphi(t) = \frac{\psi(t)}{\sqrt{1-t^2}}$. After introducing $t = \sin\theta$, $x = \sin\eta$, the integral equation becomes

(3) $K(\sin\eta) = -\frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\psi(\sin\theta)\, d\theta}{\sin\theta - \sin\eta}$ with

(3a) $\int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \psi(\sin\theta)\, d\theta = 0$.

With the points $\eta_i = -\frac{11\pi}{20} + i\,\frac{\pi}{10}$, $i = 1, 2, \ldots, 10$, and similarly $\theta_j = -\frac{11\pi}{20} + j\,\frac{\pi}{10}$, we can express the integral equation in the form

(4) $$K_i = -\frac{1}{10}\left[\sum_{\substack{j=1 \\ j\neq i}}^{10} \frac{\psi_j}{\sin\theta_j - \sin\eta_i} + \psi_i\,\frac{\sin\eta_i}{2\cos\eta_i} + \psi_i'\right]$$

for $i = 1, 2, \ldots, 10$ and

(4a) $\frac{\pi}{10}\sum_{j=1}^{10}\psi_j = 0$, where $K_i = K(\sin\eta_i)$ and $\psi_j = \psi(\sin\theta_j)$.

We evaluated the principal value integral by expanding in the interval $\eta_i - \frac{\pi}{20} \le \theta \le \eta_i + \frac{\pi}{20}$, to first order in $(\theta - \eta_i)$. In this process the ten unknown derivatives $\psi_j' = \psi'(\sin\theta_j)$ are introduced. The eleven equations (4) and (4a) are supplemented by the nine compatibility conditions

(4b) $$\psi_{i+1} - \psi_i = \frac{\pi}{20}\left[\psi_i' + \psi_{i+1}'\right]$$

for $i = 1, 2, \ldots, 9$. Because of the simple form of equations (4) and (4b) it is easy to eliminate the unknown derivative algebraically. We then are left with a system of ten linear equations for the unknowns ψ_i, $i = 1, 2, \ldots, 10$.

A sample calculation was performed for the function $K(x) = 1$. The resulting exact solution is given by $\varphi(t) = -\frac{t}{\sqrt{1-t^2}}$ and the accuracy of our numerical solution is three significant figures. (See table below.)

Method B: Since it does not appear feasible to generalize the finite difference method described above, we are examining the following scheme.

We let

(5) $$\varphi(t) = \frac{1}{\sqrt{1-t^2}}\left[a_o + a_1 t + a_2 t^2 + a_n t^n\right] .$$

We insert (5) in (2) and (2a) and determine $a_o, \ldots, a_n$

by the least squares criterion that they minimize

$$I(a_o, \ldots, a_n) = \int_{-1}^{+1} \left[K(x) + \frac{1}{\pi} \int_{-1}^{1} \frac{\varphi(t)}{t-x}\, dt\right]^2 P(x)dx \quad ,$$

where $P(x)$ is a non-negative weight. Method B, if successful, would be rather easily adaptable to problems in two dimenions.

Table of Finite Difference Solution
for $K(x) = 1$

t	$\varphi(t)$ computed	$\varphi(t)$ exact
$t_1 = \sin(-81)$	+ 6.3085133	+ 6.31375131
$t_2 = \sin(-63)$	+ 1.96098235	+ 1.96261049
$t_3 = \sin(-45)$	+ 0.99917162	+ 1.0
$t_4 = \sin(-27)$	+ 0.50910373	+ 0.50952545
$t_5 = \sin(-9)$	+ 0.15825380	+ 0.1583844
$t_6 = \sin(9)$	- 0.15825380	- 0.15838444
$t_7 = \sin(27)$	- 0.50910373	- 0.50952545
$t_8 = \sin(45)$	- 0.99917162	- 1.0
$t_9 = \sin(63)$	- 1.96098235	- 1.96261049
$t_{10} = \sin(81)$	- 6.3085133	- 6.31375131

Problem No. 1.28: Non-linear buckling of spherical shells under uniform external pressure (Dimples)

Investigators: H. J. Greenberg, H. B. Keller, E. Reiss, M. Weissner

It is well known experimentally that a thin spherical shell becomes unstable and buckles under external lateral pressure in a manner entirely at variance with the results of the linear buckling theory of elasticity. Von Karman and Tsien, Friedrichs, Tsien, and Altschuler have investigated this problem as one in the non-linear theory of elasticity with small strains. In the majority of this work the treatments were based on strain energy considerations. Although none of these attempts is really satisfactory, they do give a qualitative picture of the highly non-linear character of the deformation.

More recently, Kaplan and Fung presented a theoretical and experimental treatment of this problem. They confined their attention to shallow spherical shells. These shells may be considered as separate structural entities, or as representing the region of an entire sphere where the buckling occurs. The theoretical approach employed by Kaplan and Fung was to solve the governing differential equations --- a pair of ordinary second order non-linear differential equations --- by expanding all of the variables in powers of the center deflection and equating coefficients of equal power. This results in a sequence of linear

equations. Unfortunately, solutions to these equations could only be obtained for a small range of parameters. However, the experimental results revealed an interesting behavior in the buckling loads and modes of deformation with respect to certain parameters of the shell.

The Dimples Project is concerned with solving the governing differential equations for shallow spherical shells by power series expansions as introduced by Friedrichs and Stoker in their treatment of buckling of circular plates. These equations depend upon two parameters. One of these parameters is related to the external pressure, while the other depends upon the dimensions of the shell. The equations are solved for several ranges of the parameters under boundary conditions corresponding to a fixed edge. It is interesting to note that when the experimental results of Kaplan and Fung are interpreted in terms of these parameters, there is an improved correlation of their results as well as a reduction in the scatter of the data.

The technique of solution is to expand the dependent variables in power series in terms of the independent variable (polar angle). Substitution of these series into the differential equations yields a recurrence relation, so that all the coefficients may be expressed in terms of the first coefficient in each series. Satisfaction of the boundary conditions at the fixed edge results in non-linear algebraic equations in the coefficients. From the recurrence

relations these equations depend only on the first coefficients. These algebraic equations are then solved by an iteration scheme based on a Newton-Raphson technique. The computation of coefficients and the iteration scheme are carried out on the Univac.

Thus far, the computations have yielded the following information: Load vs, deflection, change in curvature, and stress, all at the center for the deformation up to the initial buckling load. These computations are for a rather wide range of the dimensional parameter. The results are in excellent quantitative (in many cases) as well as qualitative agreement with the experimental results of Kaplan and Fung. In addition, other interesting and unusual behaviors have been revealed. To obtain a complete description of the entire deformation a code is now being written to obtain deflection, slope, and bending and membrane stresses as functions of the independent variable for all values of the parameters. Furthermore, an attempt is under way to obtain the post-buckling behavior of the shell.

It is hoped that the results of these computations will give some indication regarding the location and character of whatever boundary layer effects may exist.

Problem No. 1.29: Underwater explosion bubble (Trouble)

Investigators: L. Fulkerson, H. B. Keller

A number of approximate theories of the oscillation of an underwater explosion bubble have been presented. The basis of most of these are the assumptions of incompressibility of the water, homogeneity of the gas bubble, and neglect of gravity and free surface effects. The first of the above assumptions has been relaxed in some theories and replaced by allowing only sonic disturbances in the water (as in Problem 1.13). As a verification of these theories we are now undertaking a direct numerical integration of the original hydrodynamical equations neglecting only gravity and the free surface.

The exploded weapon is initially replaced by a homogeneous sphere of high pressure gas with a polytropic equation of state. The surrounding water, initially homogeneous and of infinite extent, has the usual polytropic equation of state and ambient pressure characteristic of any desired depth. The numerical integration, starting from the above configuration, is intended to follow the bubble radius through the first few oscillations. It also presents the successive shocks and rarefactions sent into the water and bubble.

Problem No. 1.32: Mapping problem

Investigator: J. Moser, P. Ungar

This program has as its aim the investigation of an area-preserving mapping of a simple algebraic nature in the large. We are interested in studying the influence of a particular type of nonlinearity which is of importance in problems connected with the design of the FFAG synchrotron.

The computed example is a mapping of the simple form

$$x_1 = (x + y^3) \cos \alpha + y \sin \alpha$$

$$y_1 = -(x + y^3) \sin \alpha + y \cos \alpha \quad .$$

The problem is to find regions of stability for the mapping. This question is solved in a small neighborhood of the origin, but the behavior of the image points of the iterated mapping in a large region is completely unknown.

Problem No. 1.33: Binary mixtures (Swish)

Investigator: E. L. Rubin

One of the fundamental problems in theoretical investigations of the liquid state is the determination of the radial distribution function, the probability of finding two molecules separated by a distance r. The problem has been formally solved subject to certain approximations by Kirkwood and in a slightly different but equivalent way by Born and Green. The equations of Born and Green have been generalized to two components and this Univac calculation is being used to investigate some theoretically predictable properties of the two component system. It is believed that the roots of a certain transcendental equation will yield the temperature and density at which condensation first takes place.

NYU
NYO-
7690 C.1

N. Y. U. A. E. C. Computing
Facility.

Annual summary report.
1955-56.